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Liouville geometry of classical thermodynamics

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ABSTRACT

In the contact-geometric formulation of classical thermodynamics distinction is made between the energy and entropy representation. This distinction can be resolved by taking homogeneous coordinates for the intensive variables. It results in a geometric formulation on the cotangent bundle of the manifold of extensive variables, where all geometric objects are homogeneous in the cotangent variables. The resulting geometry based on the Liouville form is studied in depth. Additional homogeneity with respect to the extensive variables, corresponding to the classical Gibbs-Duhem relation, is treated within the same geometric framework.

1. Introduction

Starting from Gibbs' fundamental thermodynamic relation, *contact geometry* has been recognized as a natural framework for the geometric formulation of classical thermodynamics since the early 1970s [21]. This spurred a series of papers; see e.g. [29–34,4,19,11,13,16,8,26,6,17,35,23,39,10,12], and [7] for a recent introduction and survey. Other geometric work emphasizing the variational formulation of thermodynamics includes [28,15].

On the other hand, as discussed in [5], the contact-geometric formulation of thermodynamics makes a distinction between the energy and the entropy representation of the same thermodynamic system. By itself this need not be considered as a major flaw since the two representations are conformally equivalent. Nevertheless, as shown in [5], and later in [36,27,37], an attractive point of view that is *merging* the energy and entropy representation is offered by the extension of contact manifolds to *symplectic* manifolds. Compared with the odd-dimensional contact manifold this even-dimensional symplectic manifold has one more degree of freedom, called a gauge variable in [5]. From a thermodynamics perspective it amounts to replacing the intensive variables by their *homogeneous coordinates*. In fact, this *symplectization* of contact manifolds is rather well-known in differential geometry [2,25,3]; dating back to [20]. As argued in [37], the extension of contact manifolds to symplectic manifolds, apart from unifying the energy and entropy representations, offers additional advantages for the geometric formulation of thermodynamics as well. First, it yields a clear distinction between the extensive and intensive variables of the thermodynamic system. Secondly, it enables the definition of *port-thermodynamic systems*, which are

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thermodynamic systems that interact with their environment via either *power* or *entropy flow* ports. Finally, symplectization has *computational* benefits; as was already argued before by Arnold [3,4].

The present paper aims at providing an in-depth treatment of the resulting geometry of thermodynamic systems, continuing the earlier investigations in [36,37] and building upon [2,3,25]. Starting point are cotangent bundles without zero section, endowed with their natural one-form; called the *Liouville form* (sometimes also called the *Poincaré-Liouville form*). Instead of considering the symplectic geometry derived from the symplectic form $\omega = d\alpha$, where α is the Liouville form, geometric objects will be defined that are based solely on this Liouville form. The resulting geometry is called *Liouville geometry*. In particular, it will be shown how a particular class of Lagrangian submanifolds (called Liouville submanifolds) can be defined as maximal submanifolds on which the Liouville form is zero. Furthermore, a particular type of Hamiltonian vector fields is defined leaving the Liouville form invariant. All these geometric objects have the property that they are *homogeneous* in the cotangent variables. As a result they are in one-to-one correspondence with objects on the underlying contact manifold (of one dimension less). We will study in detail the generating functions of Liouville submanifolds and the homogeneous Hamiltonian functions of this special type of Hamiltonian vector fields, and relate them to their contact-geometric counterparts. Continuing upon [37] it will be shown how this leads to the definition of a port-thermodynamic system, and its projection to the contact manifold. Finally we will focus on an *additional* homogeneity, which is present in some thermodynamic systems, corresponding to homogeneity in the *extensive* variables. This leads to a new geometric view on the classical Gibbs-Duhem relation, and a subsequent projection from the contact manifold to an even-dimensional space.

The rest of the paper is structured as follows. In Section 2 it is explained, using the example of a simple gas, how macroscopic thermodynamics leads to the study of cotangent bundles over the base space of extensive variables, with cotangent variables being the homogeneous coordinates for the intensive variables. The resulting Liouville geometry of a general cotangent bundle without zero section, and its projection to contact geometry, is studied in Section 3. Then Section 4 provides the definition of port-thermodynamic systems using Liouville geometry, and its projection to a contact-geometric description. Section 5 discusses homogeneity with respect to the extensive variables, and the resulting geometric formalization of the Gibbs-Duhem relation. Finally, Section 6 contains the conclusions.

2. From thermodynamics to contact and Liouville geometry

In this section we will motivate how classical thermodynamics, starting from Gibbs' thermodynamic relation, naturally leads to contact geometry, and how by considering homogeneous coordinates for the intensive variables this results in Liouville geometry.

2.1. From Gibbs' fundamental thermodynamic relation to contact geometry

Consider a simple thermodynamic system such as a mono-phase, single constituent, gas in a confined compartment with volume V and pressure P at temperature T. It is well-known that the *state properties* of the gas are described by a 2-dimensional submanifold of the ambient space $\mathbb{R}^5$ (the *thermodynamic phase space*) with coordinates E (energy), S (entropy), V, P, and T. Such a submanifold characterizes the properties of the gas (e.g., an ideal gas, or a Van der Waals gas), and all of them share the following property. Define the *Gibbs one-form* on the thermodynamic phase space $\mathbb{R}^5$ as

$$\theta := dE - TdS + PdV \tag{1}$$

Then θ is *zero* restricted to the submanifold characterizing the state properties. This is called *Gibbs' fundamental thermodynamic relation*. It implies that the *extensive* variables E, S, V and the *intensive* variables T, P are related in a specific way. Geometrically this is formalized by noting that the Gibbs one-form θ defines a *contact form* on $\mathbb{R}^5$, and that any submanifold L capturing the state properties of the thermodynamic system is a submanifold of maximal dimension restricted to which the contact form θ is zero. Such submanifolds are called *Legendre submanifolds* of the *contact manifold* $(\mathbb{R}^5, \theta)$.

By expressing the extensive variable E as a function $E = E(S, V)$ of the two remaining extensive variables S and V, Gibbs' fundamental relation implies that the Legendre submanifold L specifying the state properties is given as

$$L = \{(E, S, V, T, P) \mid E = E(S, V), T = \frac{\partial E}{\partial S}, -P = \frac{\partial E}{\partial V}\} \tag{2}$$

Hence L is completely described by the energy function $E(S, V)$, whence the name *energy representation* for (2). On the other hand, there are other ways to represent L. If L is parametrizable by the variables T, V (instead of S, V as in (2)), then one defines the *partial Legendre transform* of $E(S, V)$ with respect to S as

$$A(T, V) := E(S, V) - TS, \quad T = \frac{\partial E}{\partial S}(S, V), \tag{3}$$

where S is solved from $T = \frac{\partial E}{\partial S}(S, V)$. Then L is also described as

$$L = \{(E, S, V, T, P) \mid E = A(T, V) - T\frac{\partial A}{\partial T}, S = -\frac{\partial A}{\partial T}, -P = \frac{\partial A}{\partial V}\} \tag{4}$$

A is known as the *Helmholtz free energy*, and is one of the thermodynamic potentials derivable from the energy function $E(S,V)$; see e.g. [14]. Two other possible parametrizations of L (namely by S,P, respectively by T,P) correspond to the thermodynamic potentials known as the enthalpy $H(S,P)$ and the Gibbs' free energy $G(T,P)$, resulting in similar expressions for L.

In general [2,25], a *contact manifold* (M,θ) is an odd-dimensional manifold equipped with a *contact form* θ. A one-form θ on a $(2n+1)$-dimensional manifold M is a contact form if and only if around any point in M we can find coordinates $(q_0,q_1,\cdots,q_n,\gamma_1,\cdots,\gamma_n)$ for M, called *Darboux coordinates*, such that

$$\theta = dq_0 - \sum_{j=1}^{n} \gamma_j dq_j \tag{5}$$

Equivalently, θ is a contact form if $\theta \wedge (d\theta)^n$ is nowhere zero on M. A *Legendre submanifold* of a contact manifold (M,θ) is a submanifold of maximal dimension restricted to which the contact form θ is zero. The dimension of any Legendre submanifold of a $(2n+1)$-dimensional contact manifold is equal to n.

In fact, throughout this paper we will use the slightly *generalized definition* of a contact manifold as given in e.g. [2], where the contact form θ *is only required to be defined locally*. What counts is the *contact distribution*; the $2n$-dimensional subspace of the tangent space at any point of M defined by the *kernel* of the contact form θ at this point. This turns out to be the appropriate concept for the thermodynamic phase space being a contact manifold.[1]

Apart from the above parametrizations of the Legendre submanifold L, corresponding to an energy function $E(S,V)$ and its Legendre transforms, there is still *another* way of describing L. This alternative, although very similar, option is directly motivated from a modeling point of view. Namely, often thermodynamic systems are formulated by listing the *balance laws* for all the extensive variables apart from the entropy S, and then expressing S as a function $S=S(E,V)$. This leads to the *entropy representation* of the submanifold $L \subset \mathbb{R}^5$, given as

$$L := \{(E,S,V,T,P) \mid S = S(E,V), \frac{1}{T} = \frac{\partial S}{\partial E}, \frac{P}{T} = \frac{\partial S}{\partial V}\} \tag{6}$$

Furthermore, analogously to the energy representation case, partial Legendre transform of $S(E,V)$ leads to other thermodynamic potentials. Geometrically the entropy representation corresponds to the *modified* Gibbs one-form

$$\widetilde{\theta} := dS - \frac{1}{T}dE - \frac{P}{T}dV, \tag{7}$$

which is obtained from the original Gibbs form θ in (1) by division by $-T$ (called *conformal equivalence*). In this way the Gibbs fundamental relation is rewritten as $\widetilde{\theta}|_L = 0$, and the intensive variables, instead of $-P,T$, now become $\frac{1}{T}, \frac{P}{T}$.

2.2. From contact to Liouville geometry

The contact-geometric view on thermodynamics, directly motivated by Gibbs' fundamental thermodynamic relation, raises two issues:
(1) Switching from the energy representation $E=E(S,V)$ to the entropy representation $S=S(E,V)$ corresponds to replacing the Gibbs form θ by the modified Gibbs form $\widetilde{\theta}$ in (7), and thus leads to a *different*, although conformally equivalent, contact-geometric description.
(2) The contact-geometric description does not make an intrinsic distinction between, on the one hand, the extensive variables E,S,V and, on the other hand, the intensive variables $T,-P$ (energy representation), or $\frac{1}{T}, \frac{P}{T}$ (entropy representation). In fact,[2] given the contact form θ on $\mathbb{R}^5$ there are many choices of Darboux coordinates $q_0,q_1,q_2,\gamma_1,\gamma_2$ such that $\theta = dq_0 - \gamma_1 dq_1 - \gamma_2 dq_2$, and q_0,q_1,q_2 are *not* necessarily obtained by a transformation of the extensive variables E,S,V only.

The way to address these issues is to *extend* the contact manifold by one extra degree of freedom to a symplectic manifold, in fact a *cotangent bundle*, with an additional *homogeneity* structure. This construction is rather well-known in differential geometry; see [2,3,25] for beautiful accounts and further ramifications. Within a thermodynamics context this 'symplectization' was advocated only in [5], and then followed up in [36,37]. For a simple thermodynamic system with extensive variables E,S,V and intensive variables $T,-P$, the construction amounts to replacing the intensive variables $T,-P$ in energy representation by their *homogeneous coordinates* p_E,p_S,p_V with $p_E \neq 0$, i.e.,

$$T = \frac{p_S}{-p_E}, \quad -P = \frac{p_V}{-p_E} \tag{8}$$

[1] Contact manifolds for which the contact form θ is defined *globally* are sometimes called *exact* contact manifolds.
[2] Note on the other hand that in the *specific* contact manifold description of $\mathbb{R}^5$ as the space of 1-jets of functions of S,V the special role of the extensive variables *is* retained.

Equivalently, the intensive variables $\frac{1}{T}, \frac{P}{T}$ in the *entropy representation* are represented as

$$\frac{1}{T} = \frac{p_E}{-p_S}, \; \frac{P}{T} = \frac{p_V}{-p_S} \tag{9}$$

with $p_S \neq 0$. This means that the *two* contact forms $\theta = dE - TdS + PdV$ and $\widetilde{\theta} = dS - \frac{1}{T}dE - \frac{P}{T}dV$ are replaced by the *single* symmetric expression

$$\alpha := p_E dE + p_S dS + p_V dV. \tag{10}$$

The one-form α is nothing else than the canonical *Liouville one-form* on the cotangent bundle $T^*\mathbb{R}^3$, with $\mathbb{R}^3$ the space of extensive variables E, S, V. As a result the thermodynamic phase space $\mathbb{R}^5$ has been replaced by $T^*\mathbb{R}^3$. More precisely, by definition of homogeneous coordinates the vector (p_E, p_S, p_V) is different from the zero vector, and hence the space with coordinates E, S, V, p_E, p_S, p_V is actually the cotangent bundle $T^*\mathbb{R}^3$ *minus* its zero section; denoted as $\mathcal{T}^*\mathbb{R}^3$.

Any 2-dimensional Legendre submanifold $L \subset \mathbb{R}^5$ describing the state properties is now replaced by a 3-dimensional submanifold $\mathcal{L} \subset \mathcal{T}^*\mathbb{R}^3$, given as

$$\mathcal{L} = \{(E, S, V, p_E, p_S, p_V) \in \mathcal{T}^*\mathbb{R}^3 \mid (E, S, V, \frac{p_S}{-p_E}, \frac{p_V}{-p_E}) \in L\} \tag{11}$$

It turns out that $\mathcal{L}$ is a *Lagrangian submanifold* of $\mathcal{T}^*\mathbb{R}^3$ with symplectic form $\omega := d\alpha$; however with an additional *homogeneity* property. Namely, whenever $(E, S, V, p_E, p_S, p_V) \in \mathcal{L}$, then also $(E, S, V, \lambda p_E, \lambda p_S, \lambda p_V) \in \mathcal{L}$, for any non-zero $\lambda \in \mathbb{R}$. Such Lagrangian submanifolds turn out to be fully characterized as maximal manifolds restricted to which the Liouville one-form $\alpha = p_E dE + p_S dS + p_V dV$ is zero, and will thus be called *Liouville submanifolds* of $\mathcal{T}^*\mathbb{R}^3$.

As we will see in the next section the extension of contact manifolds to cotangent bundles, replacing the intensive variables by their homogeneous coordinates, also leads to a natural homogeneous Hamiltonian dynamics on the extended space $\mathcal{T}^*\mathbb{R}^3$. This does not only facilitate the analysis, but has computational advantages as well [3,4]. In fact, all computations become the standard operations on cotangent bundles and of Hamiltonian dynamics. In the words of Arnold [3] (p. 5): one is advised to calculate symplectically (but to think rather in contact geometry terms). Examples of computational benefits are the somewhat involved expressions of contact vector fields (39) and their Jacobi brackets, as compared to standard expressions of Hamiltonian vector fields and Poisson brackets of Hamiltonians. Furthermore, the Jacobi bracket does not satisfy the Leibniz rule, cf. (43). These benefits are illustrated by the controllability and observability analysis of port-thermodynamic systems in [37,38].

All of the above is immediately extended from the thermodynamic phase space $\mathbb{R}^5$ to *higher-dimensional* thermodynamic phase spaces. For instance, in the case of multiple chemical species the Gibbs form θ extends to $dE - TdS + PdV - \sum_k \mu_k dN_k$, where N_k and μ_k are the mole numbers, respectively, chemical potentials, of the k-th species, $k = 1, \cdots, s$. Correspondingly, the thermodynamic phase $\mathbb{R}^5 \times \mathbb{R}^{2s}$ is replaced by the cotangent bundle without zero-section $\mathcal{T}^*\mathbb{R}^{3+s}$, with extensive variables $E, S, V, N_1, \cdots, N_s$ and Liouville form

$$p_E dE + p_S dS + p_V dV + p_1 dN_1 + \cdots + p_s dN_s, \tag{12}$$

where $\mu_1 = \frac{p_1}{-p_E}, \cdots, \mu_s = \frac{p_s}{-p_E}$.

3. Liouville geometry

This section is concerned with the general definition and analysis of geometric objects on the cotangent bundle, without zero section, that project to the underlying contact manifold. Since everything is based on the Liouville form this will be called *Liouville geometry*. In particular, we will deal with *Liouville submanifolds* and *homogeneous Hamiltonian vector fields*.

3.1. Cotangent bundles and the canonical contact manifold

In the previous section it was indicated how the thermodynamic phase space can be extended to a cotangent bundle, without its zero section, by the use of homogeneous coordinates for the intensive variables. Furthermore, it was shown how in this way the energy and entropy representation are unified, and how this provides a geometric definition of extensive and intensive variables. Conversely, in this subsection we will *start* with a general cotangent bundle without zero section, and then show how this leads to a natural *contact manifold* serving as canonical thermodynamic phase space.

Consider a thermodynamic system with its space of extensive variables, including energy E and entropy S, given by the manifold $\mathcal{Q}$. Then consider the cotangent bundle without zero section denoted by $\mathcal{T}^*\mathcal{Q}$. The *Liouville one-form* α on $\mathcal{T}^*\mathcal{Q}$ is defined as follows. Let $\eta \in \mathcal{T}^*\mathcal{Q}$, $X \in T_\eta \mathcal{T}^*\mathcal{Q}$. Then define

$$\alpha_\eta(X) := \eta(\mathrm{pr}_* X), \tag{13}$$

where $\mathrm{pr}: \mathcal{T}^*\mathcal{Q} \to \mathcal{Q}$ is the bundle projection. Furthermore $\omega := d\alpha$, with d exterior derivative, is the canonical *symplectic form* on $\mathcal{T}^*\mathcal{Q}$. Moreover, the *Euler vector field* Z is defined as the unique vector field satisfying

$$d\alpha(Z, \cdot) = \alpha \tag{14}$$

This implies $\mathbb{L}_Z\alpha = \alpha$, with $\mathbb{L}$ denoting Lie derivative.

In coordinates α, ω and Z take the following simple form. Let $\dim \mathcal{Q} = n+1$ and let $q_0, \cdots, q_n$ be local coordinates for $\mathcal{Q}$. Furthermore, let $p_0, \cdots, p_n$ be the corresponding coordinates for the cotangent spaces $T_q^*\mathcal{Q}$. Then

$$\alpha = \sum_{i=0}^{n} p_i dq_i, \quad \omega = \sum_{i=0}^{n} dp_i \wedge dq_i, \quad Z = \sum_{i=0}^{n} p_i \frac{\partial}{\partial p_i} \tag{15}$$

Based on $\mathcal{T}^*\mathcal{Q}$ we may define a *contact manifold* in the following way [2]. For each $q \in \mathcal{Q}$ and cotangent space $T_q^*\mathcal{Q}$ consider the *projective space* $\mathbb{P}(T_q^*\mathcal{Q})$, given as the set of rays in $T_q^*\mathcal{Q}$, that is, all the non-zero multiples of a non-zero cotangent vector. Thus the projective space $\mathbb{P}(T_q^*\mathcal{Q})$ has dimension n, and there is a canonical projection $\pi_q : \mathcal{T}_q^*\mathcal{Q} \to \mathbb{P}(T_q^*\mathcal{Q})$, where $\mathcal{T}_q^*\mathcal{Q}$ denotes the cotangent space without its zero vector. The fiber bundle of the projective spaces $\mathbb{P}(T_q^*\mathcal{Q})$, $q \in \mathcal{Q}$, over the base manifold $\mathcal{Q}$ will be denoted by $\mathbb{P}(T^*\mathcal{Q})$. Furthermore, the bundle projection obtained by considering $\pi_q : \mathcal{T}_q^*\mathcal{Q} \to \mathbb{P}(T_q^*\mathcal{Q})$ for every $q \in \mathcal{Q}$ is denoted by $\pi : \mathcal{T}^*\mathcal{Q} \to \mathbb{P}(T^*\mathcal{Q})$. As detailed in [2,3,37], $\mathbb{P}(T^*\mathcal{Q})$ defines a contact manifold of dimension $2n+1$ with locally defined contact form θ (while any other $(2n+1)$-dimensional contact manifold is locally *contactomorphic* to $\mathbb{P}(T^*\mathcal{Q})$ [2,25]). The contact manifold $\mathbb{P}(T^*\mathcal{Q})$ will serve as the canonical *thermodynamic phase space* for the thermodynamic system with space of extensive variables $\mathcal{Q}$.

Given natural coordinates $q_0, \cdots, q_n, p_0, \cdots, p_n$ for $\mathcal{T}^*\mathcal{Q}$, we may select different sets of local coordinates for $\mathbb{P}(T^*\mathcal{Q})$ and, correspondingly, different expressions for the projection $\pi : \mathcal{T}^*\mathcal{Q} \to \mathbb{P}(T^*\mathcal{Q})$. In fact, whenever $p_0 \neq 0$ we may express the projection $\pi_q : \mathcal{T}_q^*\mathcal{Q} \to \mathbb{P}(T_q^*\mathcal{Q})$ by the map

$$(p_0, p_1, \cdots, p_n) \mapsto (\gamma_1, \cdots, \gamma_n) \tag{16}$$

where

$$\gamma_1 = \frac{p_1}{-p_0}, \cdots, \gamma_n = \frac{p_n}{-p_0} \tag{17}$$

This means that

$$\alpha = p_0 dq_0 + p_1 dq_1 + \cdots + p_n dq_n = p_0\big(dq_0 - \gamma_1 dq_1 \cdots - \gamma_n dq_n\big) =: p_0\theta, \tag{18}$$

with θ a locally defined contact form on $\mathbb{P}(T^*\mathcal{Q})$. In particular this implies that the kernel of α projects under π to the kernel of θ; cf. [25] (Proposition 10.3) for a more general treatment.

The same can be done for any of the other coordinates p_i, defining different contact forms. For example, if $p_1 \neq 0$ we may express $\pi_q : \mathcal{T}_q^*\mathcal{Q} \to \mathbb{P}(T_q^*\mathcal{Q})$ also by the map

$$(p_0, p_1, \cdots, p_n) \mapsto (\widetilde{\gamma}_0, \widetilde{\gamma}_2, \cdots, \widetilde{\gamma}_n), \tag{19}$$

where

$$\widetilde{\gamma}_0 = \frac{p_0}{-p_1}, \widetilde{\gamma}_2 = \frac{p_2}{-p_1}, \cdots, \widetilde{\gamma}_n = \frac{p_n}{-p_1}, \tag{20}$$

so that

$$\alpha = p_1\big(dq_1 - \widetilde{\gamma}_0 dq_0 - \widetilde{\gamma}_2 dq_2 \cdots - \widetilde{\gamma}_n dq_n\big) =: p_1\widetilde{\theta} \tag{21}$$

In the thermodynamics context of Section 2, with $q_0 = E, q_1 = S$, and thus $p_0 = p_E, p_1 = p_S$, the first option corresponds to the *energy representation* and the second to the *entropy representation*.

Importantly, there is a direct *correspondence* between all geometric objects (functions, Legendre submanifolds, vector fields) on the contact manifold $\mathbb{P}(T^*\mathcal{Q})$ with the same objects on $\mathcal{T}^*\mathcal{Q}$ endowed with an additional homogeneity property in the p variables. A key element in this is Euler's theorem on homogeneous functions; see e.g. [37].

Definition 3.1. Let $r \in \mathbb{Z}$. A function $K : \mathcal{T}^*\mathcal{Q} \to \mathbb{R}$ is called homogeneous[3] of degree r in p if

$$K(q, \lambda p) = \lambda^r K(q, p), \quad \text{for all } \lambda \neq 0 \tag{22}$$

[3] Note that in coordinate-free language $K : \mathcal{T}^*\mathcal{Q} \to \mathbb{R}$ is homogeneous of degree 0 in p if and only if $\mathbb{L}_Z K = 0$, and homogeneous of degree 1 in p if and only if $\mathbb{L}_Z K = K$, where Z is the Euler vector field and $\mathbb{L}$ denotes Lie derivation.

Theorem 3.2 *(Euler's homogeneous function theorem). A differentiable function $K : \mathcal{T}^*\mathcal{Q} \to \mathbb{R}$ is homogeneous of degree r in p if and only if*

$$\sum_{i=0}^{n} p_i \frac{\partial K}{\partial p_i}(q,p) = rK(q,p), \quad \text{for all } (q,p) \in \mathcal{T}^*\mathcal{Q} \tag{23}$$

Moreover, if K is homogeneous of degree r in p, then all its partial derivatives $\frac{\partial K}{\partial p_i}(q,p), i = 0, 1, \cdots, n$, are homogeneous of degree $r-1$ in p.

Until Section 5 homogeneity will always refer to homogeneity in the p-variables; hence till then we often simply talk about 'homogeneity'.

Obviously, the functions $K : \mathcal{T}^*\mathcal{Q} \to \mathbb{R}$ that are homogeneous of degree 0 in p are those functions which project under π to functions on $\mathbb{P}(T^*\mathcal{Q})$, i.e., $K = \pi^*\widehat{K}$ with $\widehat{K} : \mathbb{P}(T^*\mathcal{Q}) \to \mathbb{R}$. In the next two subsections we will consider two more geometric objects which project to $\mathbb{P}(T^*\mathcal{Q})$.

3.2. Liouville submanifolds

Legendre submanifolds of the canonical thermodynamic phase space $\mathbb{P}(T^*\mathcal{Q})$ are in one-to-one correspondence with Liouville submanifolds[4] of $\mathcal{T}^*\mathcal{Q}$, defined as follows.

Definition 3.3. A submanifold $\mathcal{L} \subset \mathcal{T}^*\mathcal{Q}$ is called a *Liouville submanifold* if the Liouville form α restricted to $\mathcal{L}$ is zero and $\dim \mathcal{L} = \dim \mathcal{Q}$.

Recall that $\mathcal{L}$ is a *Lagrangian* submanifold of $\mathcal{T}^*\mathcal{Q}$ if $\omega = d\alpha$ is zero on $\mathcal{L}$ and $\dim \mathcal{L} = \dim \mathcal{Q}$ (or, equivalently, ω is zero on $\mathcal{L}$ and $\mathcal{L}$ is maximal with respect to this property.) The following proposition shows that Liouville submanifolds are actually Lagrangian submanifolds of $\mathcal{T}^*\mathcal{Q}$ with an additional homogeneity property.

Proposition 3.4. *$\mathcal{L} \subset \mathcal{T}^*\mathcal{Q}$ is a Liouville submanifold if and only if $\mathcal{L}$ is a Lagrangian submanifold of the symplectic manifold $(\mathcal{T}^*\mathcal{Q}, \omega)$ with the property that*

$$(q,p) \in \mathcal{L} \Rightarrow (q, \lambda p) \in \mathcal{L} \tag{24}$$

for every $0 \neq \lambda \in \mathbb{R}$.

Proof. First of all note that the homogeneity property (24) is equivalent to *tangency* of the Euler vector field Z to $\mathcal{L}$.
(Only if) By Palais' formula (see e.g. [1], Proposition 2.4.15)

$$d\alpha(X_1, X_2) = \mathbb{L}_{X_1}(\alpha(X_2)) - \mathbb{L}_{X_2}(\alpha(X_1)) - \alpha([X_1, X_2]) \tag{25}$$

for any two vector fields X_1, X_2. Hence, for any X_1, X_2 tangent to $\mathcal{L}$ we obtain $d\alpha(X_1, X_2) = 0$, implying that $\mathcal{L}$ is a Lagrangian submanifold. Furthermore, by (14)

$$d\alpha(Z, X) = \alpha(X) = 0, \tag{26}$$

for all vector fields X tangent to $\mathcal{L}$. Because $\mathcal{L}$ is a Lagrangian submanifold this implies that Z is tangent to $\mathcal{L}$ (since a Lagrangian submanifold is a *maximal* submanifold restricted to which $\omega = d\alpha$ is zero.)
(If). If $\mathcal{L}$ is Lagrangian and satisfies (24), then Z is tangent to $\mathcal{L}$, and thus (26) holds for all vector fields X tangent to $\mathcal{L}$, implying that α is zero restricted to $\mathcal{L}$. ∎

Remark 3.5. It also follows that $\mathcal{L} \subset \mathcal{T}^*\mathcal{Q}$ is a Liouville submanifold if and only if it is a *maximal* submanifold on which α is zero.

Liouville submanifolds of $\mathcal{T}^*\mathcal{Q}$ are in one-to-one correspondence with *Legendre submanifolds* of the contact manifold $\mathbb{P}(\mathcal{T}^*\mathcal{Q})$. Recall that a submanifold of a $(2n+1)$-dimensional contact manifold is a Legendre submanifold [2,25] if the (locally defined) contact form θ is zero restricted to it, and its dimension is equal to n (the maximal dimension of a submanifold on which θ is zero).

[4] Previously [37] called *homogeneous Lagrangian submanifolds*.

Proposition 3.6 *([25], Proposition 10.16, [37]). Consider the projection $\pi : \mathcal{T}^*\mathcal{Q} \to \mathbb{P}(T^*\mathcal{Q})$. Then $\widehat{\mathcal{L}} \subset \mathbb{P}(T^*\mathcal{Q})$ is a Legendre submanifold if and only if $\mathcal{L} := \pi^{-1}(\widehat{\mathcal{L}}) \subset \mathcal{T}^*\mathcal{Q}$ is a Liouville submanifold. Conversely, any Liouville submanifold $\mathcal{L} \subset \mathcal{T}^*\mathcal{Q}$ is of the form $\pi^{-1}(\widehat{\mathcal{L}})$ for some Legendre submanifold $\widehat{\mathcal{L}} \subset \mathbb{P}(T^*\mathcal{Q})$.*

This also implies a one-to-one correspondence between *generating functions* of Legendre submanifolds $\widehat{\mathcal{L}} \subset \mathbb{P}(T^*\mathcal{Q})$ and generating functions of Liouville submanifolds $\mathcal{L} \subset \mathcal{T}^*\mathcal{Q}$ with $\pi^{-1}(\widehat{\mathcal{L}}) = \mathcal{L}$. Recall from [25,2] that any Legendre submanifold $\widehat{\mathcal{L}} \subset \mathbb{P}(T^*\mathcal{Q})$ with Darboux coordinates $q_0, q_1, \cdots, q_n, \gamma_1, \cdots, \gamma_n$ can be represented as

$$\widehat{\mathcal{L}} = \{(q_0, q_1, \cdots, q_n, \gamma_1, \cdots, \gamma_n) \mid q_0 = \widehat{F} - \gamma_J \frac{\partial \widehat{F}}{\partial \gamma_J}, \, q_J = -\frac{\partial \widehat{F}}{\partial \gamma_J}, \, \gamma_I = \frac{\partial \widehat{F}}{\partial q_I}\} \tag{27}$$

for some disjoint partitioning $\{1, \cdots, n\} = I \cup J$ and some function $\widehat{F}(q_I, \gamma_J)$, called a *generating function* for $\widehat{\mathcal{L}}$. Here γ_J is the vector with elements $\gamma_\ell = \frac{p_\ell}{-p_0}, \ell \in J$, and $\gamma_J \frac{\partial \widehat{F}}{\partial \gamma_J}$ is shorthand notation for $\sum_{\ell \in J} \gamma_\ell \frac{\partial \widehat{F}}{\partial \gamma_\ell}$. Conversely any submanifold $\widehat{\mathcal{L}}$ as given in (27), for any partitioning $\{1, \cdots, n\} = I \cup J$ and function $\widehat{F}(q_I, \gamma_J)$, is a Legendre submanifold. This implies that the corresponding Liouville submanifold $\mathcal{L} = \pi^{-1}(\widehat{\mathcal{L}})$ is given as

$$\mathcal{L} = \{(q_0, \cdots, q_n, p_0, \cdots, p_n) \mid q_0 = -\frac{\partial F}{\partial p_0}, \, q_J = -\frac{\partial F}{\partial p_J}, \, p_I = \frac{\partial F}{\partial q_I}\}, \tag{28}$$

where

$$F(q_I, p_0, p_J) := -p_0 \widehat{F}(q_I, \frac{p_J}{-p_0}) \tag{29}$$

This is immediately verified by exploiting the identities

$$\begin{aligned} -\frac{\partial F}{\partial p_0} &= \widehat{F}(q_I, -\frac{p_J}{p_0}) + p_0 \frac{\partial \widehat{F}}{\partial \gamma_J}(q_I, -\frac{p_J}{p_0}) \frac{p_J}{p_0^2} = \widehat{F}(q_I, \gamma_J) - \gamma_J \frac{\partial \widehat{F}}{\partial \gamma_J} \\ \frac{\partial F}{\partial p_J} &= -p_0 \frac{\partial \widehat{F}}{\partial \gamma_J} \cdot \frac{1}{-p_0} = \frac{\partial \widehat{F}}{\partial \gamma_J}, \quad \frac{\partial F}{\partial q_I} = -p_0 \frac{\partial \widehat{F}}{\partial q_I} = -p_0 \gamma_I = p_I \end{aligned} \tag{30}$$

Thus $F(q_I, p_0, p_J)$ in (29) is a generating function of $\mathcal{L}$. Conversely, any Liouville submanifold as in (28) for some p_0 (possibly after renumbering the index set $\{0, 1, \cdots, n\}$) and generating function F as given in (29) for some $\widehat{F}(q_I, \gamma_J)$, with $I \cup J = \{1, \cdots, n\}$ and $\gamma_J = -\frac{p_J}{p_0}$ defines a Liouville submanifold of $\mathcal{T}^*\mathcal{Q}$.

Note that the generating function $F(q_I, p_0, p_J) = -p_0 \widehat{F}(q_I, \frac{p_J}{-p_0})$ as in (29) is *homogeneous of degree* 1 in p. The correspondence (29) between the generating function $F(q_I, p_0, p_J)$ of the Liouville submanifold $\mathcal{L} = \pi^{-1}(\widehat{\mathcal{L}})$ and the generating function $\widehat{F}(q_I, \gamma_J)$ of the Legendre submanifold $\widehat{\mathcal{L}}$ is of a well-known type in the theory of homogeneous functions. Indeed, for any function $K(q, p)$ that is homogeneous of degree 1 in p, we can define

$$\widehat{K}(q, \gamma_1, \cdots, \gamma_n) := K(q, -1, \gamma_1, \cdots, \gamma_n), \tag{31}$$

implying that

$$K(q, p_0, p_1, \cdots, p_n) = -p_0 \widehat{K}(q, \frac{p_1}{-p_0}, \cdots, \frac{p_n}{-p_0}) \tag{32}$$

Finally note that the correspondence between the Liouville submanifold $\mathcal{L}$ and the Legendre submanifold $\widehat{\mathcal{L}}$ and their generating functions can be obtained for *any* numbering of the set $\{0, 1, \cdots, n\}$, and thus for any choice of p_0. This provides other coordinatizations of the *same* Legendre submanifold $\widehat{\mathcal{L}} \subset \mathbb{P}(T^*\mathcal{Q})$. The representation of $\widehat{\mathcal{L}}$ either in energy or in entropy representation is an example of this.

3.3. Homogeneous Hamiltonian and contact vector fields

For any function $K : \mathcal{T}^*\mathcal{Q} \to \mathbb{R}$ the *Hamiltonian vector field* X_K on $\mathcal{T}^*\mathcal{Q}$ is defined by the standard Hamiltonian equations

$$\dot{q}_i = \frac{\partial K}{\partial p_i}(q, p), \quad \dot{p}_i = -\frac{\partial K}{\partial q_i}(q, p), \quad i = 0, 1 \cdots, n, \tag{33}$$

or equivalently, $\omega(X_K, -) = -dK$ with $\omega = d\alpha$ the symplectic form. Furthermore, any Hamiltonian vector field X_K leaves ω invariant; i.e., $\mathbb{L}_{X_K}\omega = 0$ with $\mathbb{L}$ denoting Lie derivative.

Since $d\alpha(Z, \cdot) = \alpha$, we have $\alpha(X_K) = d\alpha(Z, X_K) = \mathbb{L}_Z K = K$. Hence a Hamiltonian K is homogeneous of degree 1 in p if and only if

$$\alpha(X_K) = K \tag{34}$$

Proposition 3.7. *If $K : \mathcal{T}^*\mathcal{Q} \to \mathbb{R}$ is homogeneous of degree 1 in p then its Hamiltonian vector field X_K satisfies*

$$\mathbb{L}_{X_K}\alpha = 0 \tag{35}$$

Conversely, if the vector field X satisfies $\mathbb{L}_X\alpha = 0$, then $X = X_K$ where the function $K := \alpha(X)$ is homogeneous of degree 1 in p.

Proof. By Cartan's formula, with i denoting contraction,

$$\mathbb{L}_X\alpha = i_X d\alpha + d i_X\alpha = i_X d\alpha + d(\alpha(X)) \tag{36}$$

If K is homogeneous of degree 1 in p then by (34) $i_{X_K}d\alpha + d(\alpha(X_K)) = -dK + dK = 0$, implying by (36) that $\mathbb{L}_{X_K}\alpha = 0$. Conversely, if $\mathbb{L}_X\alpha = 0$, then (36) yields $i_X d\alpha + d(\alpha(X))$, implying that $X = X_K$ with $K = \alpha(X)$, which by (34) is homogeneous of degree 1 in p. ■

Thus the Hamiltonian vector fields with a Hamiltonian homogeneous of degree 1 in p are precisely the vector fields that leave the Liouville form α invariant. For simplicity of exposition the Hamiltonians $K : \mathcal{T}^*\mathcal{Q} \to \mathbb{R}$ that are homogeneous of degree 1 in p, and their corresponding Hamiltonian vector fields X_K, will be simply called *homogeneous* in the sequel.

Since K is homogeneous of degree 1 in p by Euler's theorem the expressions $\frac{\partial K}{\partial p_i}(q,p), i = 0, 1 \cdots, n$, are homogeneous of degree 0 in p. Hence the dynamics of the extensive variables q in the Hamiltonian dynamics (33) is invariant under scaling of the p-variables, and thus expressible as a function of q and the intensive variables γ. This implies that any homogeneous Hamiltonian vector field projects to a *contact vector field* on the thermodynamic phase space $\mathbb{P}(T^*\mathcal{Q})$, and conversely that any contact vector field on $\mathbb{P}(T^*\mathcal{Q})$ is the projection of a homogeneous Hamiltonian vector field on $\mathcal{T}^*\mathcal{Q}$. This can be made explicit by the following computations. Consider a homogeneous Hamiltonian vector field X_K. Since K is homogeneous of degree 1 in p we can write as in (32) $K(q,p) = -p_0\widehat{K}(q, \frac{p_1}{-p_0}, \cdots, \frac{p_n}{-p_0})$, with $\widehat{K}(q,\gamma)$ defined in (31). This means that the equations (33) of the Hamiltonian vector field X_K take the form

$$\begin{array}{rcll} \dot{q}_0 & = & -\widehat{K}(q,\gamma) - p_0\sum_{\ell=1}^n \frac{\partial \widehat{K}}{\partial \gamma_\ell}(q,\gamma)\cdot -\frac{p_\ell}{p_0^2} = -\widehat{K}(q,\gamma) + \sum_{\ell=1}^n \gamma_\ell \frac{\partial \widehat{K}}{\partial \gamma_\ell}(q,\gamma) & \\ \dot{q}_j & = & -p_0\frac{\partial \widehat{K}}{\partial \gamma_j}(q,\gamma)\cdot \frac{1}{-p_0} = \frac{\partial \widehat{K}}{\partial \gamma_j}(q,\gamma), & j = 1, \cdots, n \\ \dot{p}_i & = & p_0\frac{\partial \widehat{K}}{\partial q_i}(q,\gamma), & i = 0, \cdots, n \end{array} \tag{37}$$

where $\gamma_j = \frac{p_j}{-p_0}, j = 1, \cdots, n$. Combining with

$$\dot{\gamma}_j = \frac{1}{-p_0}\dot{p}_j + \frac{p_j}{p_0^2}\dot{p}_0, \quad j = 1, \cdots, n, \tag{38}$$

this yields the following projected dynamics on the contact manifold $\mathbb{P}(T^*\mathcal{Q})$ with coordinates (q,γ)

$$\begin{array}{rcll} \dot{q}_0 & = & \sum_{\ell=1}^n \gamma_\ell \frac{\partial \widehat{K}}{\partial \gamma_\ell}(q,\gamma) - \widehat{K}(q,\gamma) & \\ \dot{q}_j & = & \frac{\partial \widehat{K}}{\partial \gamma_j}(q,\gamma), & j = 1, \cdots, n \\ \dot{\gamma}_j & = & -\frac{\partial \widehat{K}}{\partial q_j}(q,\gamma) - \gamma_j\frac{\partial \widehat{K}}{\partial q_0}(q,\gamma), & j = 1 \cdots, n \end{array} \tag{39}$$

This is recognized as the *contact vector field* [25] with *contact Hamiltonian* $\widehat{K}$. Indeed, given a contact form θ the contact vector field $X_{\widehat{K}}$ with contact Hamiltonian $\widehat{K}$ is defined through the relations[5]

$$\mathbb{L}_{X_{\widehat{K}}}\theta = \rho_{\widehat{K}}\theta, \quad -\widehat{K} = \theta(X_{\widehat{K}}) \tag{40}$$

for some function $\rho_{\widehat{K}}$ (depending on $\widehat{K}$). The first equation in (40) expresses the condition that the contact vector field leaves the contact distribution (the kernel of the contact form θ) invariant. Equations (40) for $\theta = dq_0 - \gamma_1 dq_1 \cdots - \gamma_n dq_n$ and $\widehat{K}(q,\gamma)$ can be seen to yield the same equations as in (39); see [25,11] for details. Conversely, any contact vector field with contact Hamiltonian $\widehat{K}(q,\gamma)$ defines a homogeneous Hamiltonian vector field on $\mathcal{T}^*\mathcal{Q}$ with homogeneous Hamiltonian $-p_0\widehat{K}(q, \frac{p_1}{-p_0}, \cdots, \frac{p_n}{-p_0})$. As before, the coordinate expression (39) of the contact vector field depends on the numbering of the homogeneous coordinates $p_0, p_1, \cdots, p_n$; i.e., the choice of p_0. In the thermodynamics context this is again illustrated by the choice of either the energy or entropy representation (corresponding to choosing $p_0 = p_E$ or $p_0 = p_S$). Furthermore, as shown by (39) the dynamics of the extensive variables depends on the extensive variables and (part of) the intensive variables (either in energy or entropy representation).

The projectability of any homogeneous Hamiltonian vector field X_K to a vector field on $\mathbb{P}(T^*\mathcal{Q})$ also follows from the next proposition, together with the fact that the projection $\pi : \mathcal{T}^*\mathcal{Q} \to \mathbb{P}(T^*\mathcal{Q})$ is along the Euler vector field Z.

[5] Here the sign convention of [7] is followed.

Proposition 3.8. *Any homogeneous Hamiltonian vector field X_K satisfies $[X_K, Z] = 0$.*

Proof. By [1] (Table 2.4-1) and $\mathbb{L}_{X_K}\alpha = 0$

$$i_{[X_K,Z]}d\alpha = \mathbb{L}_{X_K} i_Z d\alpha - i_Z \mathbb{L}_{X_K} d\alpha = \mathbb{L}_{X_K}\alpha - i_Z d\mathbb{L}_{X_K}\alpha = 0 - 0 = 0 \tag{41}$$

Because $\omega = d\alpha$ is non-degenerate this implies $[X_K, Z] = 0$. ■

Although homogeneous Hamiltonian vector fields are in one-to-one correspondence with contact vector fields, typically *computations* for homogeneous Hamiltonian vector fields are more easy than the corresponding computations for their contact vector field counterparts. First let us note the following properties proved in [37,36].

Proposition 3.9. *Consider the Poisson bracket $\{K_1, K_2\}$ of functions K_1, K_2 on $\mathcal{T}^*\mathcal{Q}$ defined with respect to the symplectic form $\omega = d\alpha$. Then*

(a) *If K_1, K_2 are both homogeneous of degree 1 in p, then also $\{K_1, K_2\}$ is homogeneous of degree 1 in p.*
(b) *If K_1 is homogeneous of degree 1 in p, and K_2 is homogeneous of degree 0 in p, then $\{K_1, K_2\}$ is homogeneous of degree 0 in p.*
(c) *If K_1, K_2 are both homogeneous of degree 0 in p, then $\{K_1, K_2\}$ is zero.*

Using property (a) we may define the following bracket

$$\{\widehat{K}_1, \widehat{K}_2\}_J := \widehat{\{K_1, K_2\}} \tag{42}$$

where $\widehat{K}$ is the contact Hamiltonian corresponding to the homogeneous Hamiltonian K as in (40). The bracket $\{\widehat{K}_1, \widehat{K}_2\}_J$ is equal to the *Jacobi bracket* of the contact Hamiltonians $\widehat{K}_1, \widehat{K}_2$; see e.g. [25,7,2] for the somewhat complicated coordinate expression of the Jacobi bracket. The Jacobi bracket is obviously bilinear and skew-symmetric. Furthermore, since the Poisson bracket satisfies the Jacobi-identity, so does the Jacobi bracket. However, the Jacobi bracket does *not* satisfy the Leibniz rule; i.e., in general the following equality does *not* hold

$$\{\widehat{K}_1, \widehat{K}_2 \cdot \widehat{K}_3\}_J = \{\widehat{K}_1, \widehat{K}_2\}_J \cdot \widehat{K}_3 + \widehat{K}_2 \cdot \{\widehat{K}_1, \widehat{K}_3\}_J \tag{43}$$

See also [39] for additional information on the Jacobi bracket.

3.4. Hamilton-Jacobi theory of Liouville and Legendre submanifolds

Recall that any homogeneous Hamiltonian vector field X_K on $\mathcal{T}^*\mathcal{Q}$ leaves invariant the Liouville form α, and that Liouville submanifolds are maximal submanifolds on which α is zero. Since $\mathbb{L}_{X_K}\alpha = 0$ it follows that for any Liouville submanifold $\mathcal{L}$ and any time $t \in \mathbb{R}$ the evolution of $\mathcal{L}$ along the homogeneous Hamiltonian vector field X_K given by

$$\phi_t(\mathcal{L}) := \{\phi_t(z) \mid z \in \mathcal{L}\}, \tag{44}$$

where $\phi_t : \mathcal{T}^*\mathcal{Q} \to \mathcal{T}^*\mathcal{Q}$ is the flow map of X_K at time $t \geq 0$, is again a Liouville submanifold. Thus the flow of a homogeneous Hamiltonian vector field transforms the Liouville submanifold to another Liouville submanifold at any time $t \geq 0$. For example, the Liouville submanifold corresponding to an ideal gas may be continuously transformed into the Liouville submanifold of a Van der Waals gas. This point of view was explored in a contact-geometric setting in [29,30,32].

Furthermore, cf. (29), let $F(q_I, p_0, p_J) := -p_0\widehat{F}(q_I, \frac{p_J}{-p_0})$, with $I \cup J = \{1, \cdots, n\}$, be the generating function of $\mathcal{L}$, then it follows that for any $t \geq 0$ the generating function $G(q_I, p_0, p_J, t) := -p_0\widehat{G}(q_I, \frac{p_J}{-p_0}, t)$ of the transformed Liouville submanifold $\phi_t(\mathcal{L})$ satisfies the *Hamilton-Jacobi equation*

$$\begin{aligned} &\tfrac{\partial G}{\partial t} + K(q_0, q_I, -\tfrac{\partial G}{\partial p_J}, p_0, \tfrac{\partial G}{\partial q_J}, p_J) = 0 \\ &G(q_I, p_0, p_J, 0) = F(q_I, p_0, p_J) \end{aligned} \tag{45}$$

In the case of the evolution of a *general* Lagrangian submanifold under the dynamics of a *general* Hamiltonian vector field, this is classical Hamilton-Jacobi theory (see e.g. [1,2]), which directly specializes to Liouville submanifolds and to homogeneous Hamiltonian vector fields. Moreover, the generating functions $\widehat{G}(q_I, \gamma_J, t)$ of the corresponding Legendre submanifolds $\widehat{\phi_t(\mathcal{L})}$ satisfy the Hamilton-Jacobi equation (see also [8])

$$\begin{aligned} &\tfrac{\partial \widehat{G}}{\partial t} + \widehat{K}(q_0 = \widehat{G} - \gamma_J \tfrac{\partial \widehat{G}}{\partial \gamma_J}, q_J = -\tfrac{\partial \widehat{F}}{\partial \gamma_J}, \gamma_I = \tfrac{\partial \widehat{F}}{\partial q_I}) = 0 \\ &\widehat{G}(q_I, \gamma_J, 0) = \widehat{F}(q_I, \gamma_J) \end{aligned} \tag{46}$$

Note furthermore that $\widehat{\phi_t(\mathcal{L})} = \widehat{\phi}_t(\widehat{\mathcal{L}})$, where $\widehat{\phi}_t$ is the flow map at time t of the contact vector field $X_{\widehat{K}}$. This implies as well the following result concerning the *invariance* of Liouville and corresponding Legendre submanifolds, which will be one of the starting points for the definition of port-thermodynamic systems in the following section.

Proposition 3.10. *[31,25,36] Let $K : \mathcal{T}^*\mathcal{Q} \to \mathbb{R}$ be homogeneous of degree 1 in p, and let $\widehat{K} : \mathbb{P}(T^*\mathcal{Q}) \to \mathbb{R}$ be the corresponding contact Hamiltonian. Furthermore let $\mathcal{L} \subset \mathcal{T}^*\mathcal{Q}$ be a Liouville submanifold, with $\mathcal{L} = \pi^{-1}(\widehat{\mathcal{L}})$ and $\widehat{\mathcal{L}} \subset \mathbb{P}(T^*\mathcal{Q})$ the corresponding Legendre submanifold. Then the following statements are equivalent:*

1. *The homogeneous Hamiltonian vector field X_K leaves $\mathcal{L}$ invariant.*
2. *The contact vector field $X_{\widehat{K}}$ leaves $\widehat{\mathcal{L}}$ invariant.*
3. *K is zero on $\mathcal{L}$.*
4. *$\widehat{K}$ is zero on $\widehat{\mathcal{L}}$.*

4. Port-thermodynamic systems

So far the geometric description of classical thermodynamics has been concerned with the *state properties*; starting from Gibbs' fundamental relation. Since these state properties are intrinsic to any thermodynamic system, they should be respected by any dynamics (thermodynamic processes). Hence any dynamics of an actual thermodynamic system should leave invariant the Liouville and Legendre submanifold characterizing the state properties [31,33,6,37]. Furthermore, desirably this should be the case for all possible state properties of the thermodynamic system, i.e., for all Liouville and Legendre submanifolds. This suggests that the dynamics on the canonical thermodynamic phase space $\mathbb{P}(T^*Q)$ should be a *contact vector field* $X_{\widehat{K}}$, and the corresponding dynamics on $\mathcal{T}^*\mathcal{Q}$ a *homogeneous Hamiltonian vector field* X_K.

Because of its simplicity, we first focus on the homogeneous Hamiltonian description. Consider a thermodynamic system with constitutive relations (state properties) specified by a Liouville submanifold $\mathcal{L} \subset \mathcal{T}^*\mathcal{Q}$. Respecting the geometric structure means that the dynamics is a Hamiltonian vector field X_K on $\mathcal{T}^*\mathcal{Q}$, with K homogeneous of degree 1 in the p-variables. Furthermore, since the state properties captured by $\mathcal{L}$ are intrinsic to the system, the homogeneous Hamiltonian vector field X_K should leave $\mathcal{L}$ *invariant*. By Proposition 3.10 this means that the homogeneous Hamiltonian K governing the dynamics should be zero on $\mathcal{L}$. Furthermore, we will split K into two parts, i.e.,

$$K^a + K^c u, \quad u \in \mathbb{R}^m, \tag{47}$$

where $K^a : \mathcal{T}^*\mathcal{Z} \to \mathbb{R}$ is the homogeneous Hamiltonian corresponding to the *autonomous* dynamics due to internal non-equilibrium conditions, while $K^c = (K_1^c, \cdots, K_m^c)$ is a row vector of homogeneous Hamiltonians (called *control* or *interaction* Hamiltonians) corresponding to dynamics arising from *interaction with the surroundings* of the system. This second part of the dynamics will be supposed to be affinely parametrized by a vector u of *control* or *input* variables (see however [37] for an example of non-affine dependency). This means that all $(m+1)$ functions $K^a, K_1^c, \cdots, K_m^c$ are homogeneous of degree 1 in p and zero on $\mathcal{L}$.

By invoking Euler's theorem (Theorem 3.2) homogeneity of degree 1 in p means

$$\begin{aligned} K^a &= p_0 \tfrac{\partial K^a}{\partial p_0} + p_1 \tfrac{\partial K^a}{\partial p_1} + \cdots + p_n \tfrac{\partial K^a}{\partial p_n} \\ K^c &= p_0 \tfrac{\partial K^c}{\partial p_0} + p_1 \tfrac{\partial K^c}{\partial p_1} + \cdots + p_n \tfrac{\partial K^c}{\partial p_n}, \end{aligned} \tag{48}$$

where the functions $\frac{\partial K^a}{\partial p_i}$, as well as the elements of the m-dimensional row vectors of partial derivatives $\frac{\partial K^c}{\partial p_i}$, $i = 0, 1, \cdots, n$, are all homogeneous of degree 0 in the p-variables.

The class of allowable autonomous Hamiltonians K^a is further restricted by the *First and Second Law* of thermodynamics. Since the energy and entropy variables E, S are among the extensive variables $q_0, q_1, \cdots, q_n$, let us denote $q_0 = E, q_1 = S$. With this convention, the evolution of E in the autonomous dynamics X_{K^a} arising from internal non-equilibrium conditions is given by $\dot{E} = \frac{\partial K^a}{\partial p_0}$. Since by the First Law the energy of the system without interaction with the surroundings (i.e., for $u = 0$) should be *conserved*, this implies that necessarily $\frac{\partial K^a}{\partial p_0}|_{\mathcal{L}} = 0$. Similarly, $\dot{S}$ in the autonomous dynamics X_{K^a} is given by $\frac{\partial K^a}{\partial p_1}$. Hence by the Second Law necessarily $\frac{\partial K^a}{\partial p_1}|_{\mathcal{L}} \geq 0$.

These two constraints need not hold for the control (interaction) Hamiltonians K^c. In fact, the analogous terms in the control Hamiltonians may be utilized to define natural *output* variables. First option is to define the output vector as the m-dimensional row vector (p for power)

$$y_p = \frac{\partial K^c}{\partial p_0} \tag{49}$$

Then it follows that along the complete dynamics X_K on $\mathcal{L}$, with $K = K^a + K^c u$,

$$\frac{d}{dt} E = y_p u \tag{50}$$

Thus y_p is the vector of *power conjugate* outputs corresponding to the input vector u. We call the pair (u, y_p) the *power port* of the system. Similarly, by defining the output vector as the m-dimensional row vector (e for 'entropy flow')

$$y_e = \frac{\partial K^c}{\partial p_1}, \tag{51}$$

it follows that along the dynamics X_K on $\mathcal{L}$

$$\frac{d}{dt} S \geq y_e u \tag{52}$$

Hence y_e is the output vector which is conjugate to u in terms of *entropy flow*. The pair (u, y_e) is called the *flow of entropy* port of the system.

The above discussion is summarized in the following definition of a *port-thermodynamic system*.

Definition 4.1 *([37]).* Consider the manifold of extensive variables $\mathcal{Q}$. A port-thermodynamic system on $\mathcal{Q}$ is defined by a pair $(\mathcal{L}, K)$, where $\mathcal{L} \subset \mathcal{T}^*\mathcal{Q}$ is a Liouville submanifold describing the *state properties*, and $K = K^a + K^c u, u \in \mathbb{R}^m$, is a Hamiltonian on $\mathcal{T}^*\mathcal{Q}$, homogeneous of degree 1 in p, and zero restricted to $\mathcal{L}$. Furthermore, let $q = (q_0, q_1, \cdots, q_n)$ with $q_0 = E$ (energy), and $q_1 = S$ (entropy). Then K^a is required to satisfy $\frac{\partial K^a}{\partial p_0}|_{\mathcal{L}} = 0$ and $\frac{\partial K^a}{\partial p_1}|_{\mathcal{L}} \geq 0$. The *power conjugate output* vector of the port-thermodynamic system is defined as $y_p = \frac{\partial K^c}{\partial p_0}$, and the *entropy flow conjugate output* vector as $y_e = \frac{\partial K^c}{\partial p_1}$.

Note that any port-thermodynamic system on $\mathcal{T}^*\mathcal{Q}$ defines a corresponding system on the *thermodynamic phase space* $\mathbb{P}(T^*\mathcal{Q})$. Indeed, since $\mathcal{L} \subset \mathcal{T}^*\mathcal{Q}$ is a Liouville submanifold it projects to a Legendre submanifold $\widehat{\mathcal{L}} \subset \mathbb{P}(T^*\mathcal{Q})$. Furthermore, since K is homogeneous of degree 1 in p it has the form $K(q,p) = -p_0 \widehat{K}(q,\gamma)$, $\gamma_j = \frac{p_j}{-p_0}, j = 1, \cdots, n$, with $\widehat{K}(q,\gamma) = \widehat{K}^a(q,\gamma) + \widehat{K}^c(q,\gamma)u$ the contact Hamiltonian of the *energy representation*. This contact Hamiltonian $\widehat{K}$ is zero on $\widehat{\mathcal{L}}$, while the Hamiltonian dynamics X_K projects to the contact vector field $X_{\widehat{K}}$ which leaves invariant $\widehat{\mathcal{L}}$. Similarly, we can write $K(q,p) = -p_1 \widehat{\widehat{K}}(q,\tilde{\gamma})$, $\tilde{\gamma}_j = \frac{p_j}{-p_1}, j = 0, 2 \cdots, n$, with $\widehat{\widehat{K}}(q,\tilde{\gamma})$ the contact Hamiltonian of the *entropy representation*. Furthermore, by Euler's theorem both the power conjugate output y_p and the entropy flow conjugate output y_e are homogeneous of degree 0, and thus project to functions on $\mathbb{P}(T^*\mathcal{Q})$. Moreover, in the energy representation we can rewrite the power conjugate output y_p as

$$y_p = \frac{\partial K^c}{\partial p_0} = \sum_{\ell=1}^{n} \gamma_\ell \frac{\partial \widehat{K}^c}{\partial \gamma_\ell}(q,\gamma) - \widehat{K}^c(q,\gamma) \tag{53}$$

Similarly for the entropy flow conjugate output $y_e = \frac{\partial K^c}{\partial p_1} = \sum_{\ell=0,2}^{n} \tilde{\gamma}_\ell \frac{\partial \widehat{\widehat{K}}^c}{\partial \tilde{\gamma}_\ell}(q,\tilde{\gamma}) - \widehat{\widehat{K}}^c(q,\tilde{\gamma})$. Finally note that the constraints imposed on K^a by the First and Second law can be written in contact-geometric terms as

$$\begin{array}{l} \left(\sum_{\ell=1}^{n} \gamma_\ell \frac{\partial \widehat{K}^a}{\partial \gamma_\ell}(q,\gamma) - \widehat{K}^a(q,\gamma) \right) |_{\widehat{\mathcal{L}}} = 0 \\ \left(\sum_{\ell=0,2}^{n} \tilde{\gamma}_\ell \frac{\partial \widehat{\widehat{K}}^a}{\partial \tilde{\gamma}_\ell}(q,\gamma) - \widehat{\widehat{K}}^a(q,\tilde{\gamma}) \right) |_{\widehat{\mathcal{L}}} \geq 0 \end{array} \tag{54}$$

Example 4.2 *(Gas-piston-damper system).* Consider a gas in a thermally isolated compartment closed by a piston. The extensive variables are given by energy E, entropy S, volume V, and momentum of the piston π. The state properties of the system are described by the Liouville submanifold $\mathcal{L}$ with generating function (in energy representation) $-p_E \left(U(S,V) + \frac{\pi^2}{2m} \right)$, where $U(S,V)$ is the energy of the gas, and $\frac{\pi^2}{2m}$ is the kinetic energy of the piston with mass m. This defines the state properties

$$\begin{array}{rcl} \mathcal{L} & = & \{(E,S,V,\pi,p_E,p_S,p_V,p_\pi) \mid E = U(S,V) + \frac{\pi^2}{2m}, \\ & & p_S = -p_E \frac{\partial U}{\partial S}(S,V), p_V = -p_E \frac{\partial U}{\partial V}(S,V), p_\pi = -p_E \frac{\pi}{m} \} \end{array} \tag{55}$$

Assume the damper is linear with damping constant d. The dynamics of the gas-piston-damper system, with piston actuated by a force u, is given by X_K, where the homogeneous Hamiltonian $K : \mathcal{T}^*\mathbb{R}^4 \to \mathbb{R}$ is given as

$$K = p_V \frac{\pi}{m} + p_\pi \left(-\frac{\partial U}{\partial V} - d \frac{\pi}{m} \right) + p_S \frac{d(\frac{\pi}{m})^2}{\frac{\partial U}{\partial S}} + \left(p_\pi + p_E \frac{\pi}{m} \right) u, \tag{56}$$

which is zero on $\mathcal{L}$. The power conjugate output $y_p = \frac{\pi}{m}$ is the velocity of the piston. In energy representation the description projects to the thermodynamic phase space $\mathbb{P}(T^*\mathbb{R}^4) = \{(E,S,V,\pi,T,-P,v)\}$, with $\gamma_S = T$ (temperature), $\gamma_V = -P$ (pressure), and $\gamma_\pi = v$ (velocity of the piston) as follows. First note that $\mathcal{L}$ projects to the Legendre submanifold

$$\widehat{\mathcal{L}} = \{(E,S,V,\pi,T,-P,v) \mid E = U(S,V) + \frac{\pi^2}{2m}, T = \frac{\partial U}{\partial S}, -P = \frac{\partial U}{\partial V}, v = \frac{\pi}{m}\} \tag{57}$$

Furthermore, $K = -p_E \widehat{K}$ with

$$\widehat{K} = -P\frac{\pi}{m} + v\left(-\frac{\partial U}{\partial V} - d\frac{\pi}{m}\right) + T\frac{d(\frac{\pi}{m})^2}{\frac{\partial U}{\partial S}} + (v - \frac{\pi}{m})u \tag{58}$$

This yields the following dynamics of the extensive variables

$$\begin{array}{rcl} \dot{E} &=& \frac{\pi}{m}u \\ \dot{S} &=& d(\frac{\pi}{m})^2/\frac{\partial U}{\partial S} \quad (\geq 0) \\ \dot{V} &=& \frac{\pi}{m} \\ \dot{\pi} &=& -\frac{\partial U}{\partial V} - d\frac{\pi}{m} + u, \end{array} \tag{59}$$

while the intensive variables satisfy $\dot{T} = -\frac{\partial \widehat{K}}{\partial S}, -\dot{P} = -\frac{\partial \widehat{K}}{\partial V}, \dot{v} = -\frac{\partial \widehat{K}}{\partial \pi}$. Similarly for the entropy representation.

In *composite* thermodynamic systems, there is typically no *single* energy or entropy. In this case the *sum* of the energies needs to be conserved by the autonomous dynamics, and likewise the *sum* of the entropies needs to be increasing. A simple example is the following; see [37] for further information.

Example 4.3 *(Heat exchanger).* Consider two heat compartments, exchanging a heat flow through a conducting wall according to Fourier's law. Each heat compartment is described by an entropy S_i and energy E_i, $i = 1,2$, corresponding to the Liouville submanifolds

$$\mathcal{L}_i = \{(E_i, S_i, p_{E_i}, p_{S_i}) \mid E_i = E_i(S_i), p_{S_i} = -p_{E_i}E_i'(S_i)\}, \quad E_i'(S_i) \geq 0 \tag{60}$$

Taking u_i as the incoming heat flow into the i-th compartment corresponds to

$$K_i^c = p_{S_i}\frac{1}{E_i'(S_i)} + p_{E_i}, \tag{61}$$

while $K_i^a = 0$. This defines for $i = 1,2$ the flow of entropy conjugate output as $y_{ei} = \frac{1}{E_i'(S_i)}$ (reciprocal temperature). The conducting wall is described by the interconnection equations (with λ Fourier's conduction coefficient)

$$-u_1 = u_2 = \lambda(\frac{1}{y_{e1}} - \frac{1}{y_{e2}}), \tag{62}$$

relating the incoming heat flows u_i and reciprocal temperatures y_i, $i = 1,2$, at both sides of the conducting wall. This leads to (setting $E(S_1,S_2) := E_1(S_1) + E_2(S_2)$, $p_{E_1} = p_{E_2} =: p_E$, cf. [37]) the autonomous dynamics generated by the homogeneous Hamiltonian

$$K^a := K_1^c u_1 + K_2^c u_2 = \lambda\left(p_{S_1}\frac{1}{E'(S_1)} + p_{S_2}\frac{1}{E'(S_2)}\right)\left(E'(S_2) - E'(S_1)\right) \tag{63}$$

Hence the total entropy on the Liouville submanifold

$$\mathcal{L} = \{(E, S_1, S_2, p_E, p_{S_1}, p_{S_2}) | E = E_1 + E_2, p_{S_1} = -p_E E_1'(S_1), p_{S_2} = -p_E E_2'(S_2)\} \tag{64}$$

satisfies

$$\frac{d}{dt}(S_1 + S_2) = \lambda(\frac{1}{E_1'(S_1)} - \frac{1}{E_2'(S_2)})(E_2'(S_2) - E_1'(S_1)) \geq 0 \tag{65}$$

Interestingly, while the Hamiltonians in standard Hamiltonian systems (such as in mechanics) represent *energy*, the Hamiltonians K in the above examples are *dimensionless* (in the sense of dimensional analysis). This holds in general. Furthermore, it can be verified that the *contact Hamiltonian* of the projected dynamics (a contact vector field) has dimension of *power* in case of the energy representation, and has dimension of *entropy flow* in case of the entropy representation. Together with the fact that the dynamics of a thermodynamic system is captured by the dynamics *restricted* to its invariant Liouville submanifold, this underscores the fact that the *interpretation* of the Hamiltonian dynamics X_K is rather *different* from that of mechanical (or other physical) systems.

Finally, let us recall the well-known correspondence [25,2] between *Poisson brackets* of Hamiltonians K_1, K_2, and *Lie brackets* of their corresponding Hamiltonian vector fields, i.e.,

$$[X_{K_1}, X_{K_2}] = X_{\{K_1,K_2\}} \tag{66}$$

In particular, this property implies that if the homogeneous Hamiltonians K_1, K_2 are zero on the Liouville submanifold $\mathcal{L}$, and thus by Proposition 3.10 the homogeneous Hamiltonian vector fields X_{K_1}, X_{K_2} are tangent to $\mathcal{L}$, then also $[X_{K_1}, X_{K_2}]$ is tangent to $\mathcal{L}$, and therefore the Poisson bracket $\{K_1, K_2\}$ is also zero on $\mathcal{L}$. Together with Proposition 3.9 this was crucially used in the controllability and observability analysis of port-thermodynamic systems in [37,38].

5. Homogeneity in the extensive variables and Gibbs-Duhem relation

In many thermodynamic systems, when taking into account *all* extensive variables, there is an additional form of homogeneity; but now with respect to the *extensive* variables q. To start with, consider a Liouville submanifold $\mathcal{L}$ with generating function $-p_0\widehat{F}(q_1,\cdots,q_n)$, describing the state properties of a thermodynamic system. Recall that if q_0 denotes the energy variable, then $\widehat{F}(q_1,\cdots,q_n)$ equals the energy q_0 expressed as a function of the other extensive variables $q_1,\cdots,q_n$. Assume that the manifold of extensive variables $\mathcal{Q}$ is the *linear space*[6] $\mathcal{Q}=\mathbb{R}^{n+1}$. Homogeneity with respect to the extensive variables now means that the function $\widehat{F}$ is homogeneous of degree 1 in $q_1,\cdots,q_n$. This implies by Euler's theorem (Theorem 3.2) that $\widehat{F}=\sum_{j=1}^n q_j\frac{\partial \widehat{F}}{\partial q_j}$. Hence on the corresponding Legendre submanifold $\widehat{\mathcal{L}}=\pi(\mathcal{L})$ we have $\widehat{F}=\sum_{j=1}^n \gamma_j q_j$, and thus

$$d\widehat{F}=\sum_{j=1}^n \gamma_j dq_j+\sum_{j=1}^n q_j d\gamma_j \tag{67}$$

By Gibbs' relation $d\widehat{F}-\sum_{j=1}^n \gamma_j dq_j=0$ on $\widehat{\mathcal{L}}$, and hence on $\widehat{\mathcal{L}}$

$$\sum_{j=1}^n q_j d\gamma_j=0 \tag{68}$$

This is known as the *Gibbs-Duhem relation*; see e.g. [24,18]. The relation in particular implies that the intensive variables γ_j on $\widehat{\mathcal{L}}$ are *dependent*.

More generally this can be formulated in the following *geometric* way.

Definition 5.1. Let $\mathcal{Q}=\mathbb{R}^{n+1}$ with linear coordinates q. A Liouville submanifold $\mathcal{L}\subset\mathcal{T}^*\mathbb{R}^{n+1}$ is *homogeneous with respect to the extensive variables q* if

$$(q_0,q_1,\cdots,q_n,p_0,\cdots,p_n)\in\mathcal{L}\Rightarrow(\mu q_0,\mu q_1,\cdots,\mu q_n,p_0,\cdots,p_n)\in\mathcal{L} \tag{69}$$

for all $0\neq\mu\in\mathbb{R}$.

Using the same theory as exploited before for homogeneity with respect to the p-variables, cf. Proposition 3.4, homogeneity of $\mathcal{L}$ with respect to q is equivalent to the vector field $W:=\sum_{i=0}^n q_i\frac{\partial}{\partial q_i}$ being *tangent* to $\mathcal{L}$. Hence, using the same argumentation as in Proposition 3.4, not only the Liouville form $\alpha=\sum_{i=0}^n p_i dq_i$ is zero on $\mathcal{L}$, but also the one-form

$$\beta:=\sum_{i=0}^n q_i dp_i \tag{70}$$

This could be called the *generalized* Gibbs-Duhem relation.

Proposition 5.2. *The Liouville submanifold $\mathcal{L}$ is homogeneous with respect to the extensive variables q if and only if $\beta=\sum_{i=0}^n q_i dp_i$ is zero on $\mathcal{L}$. Let $\mathcal{L}$ have generating function $-p_0\widehat{F}(q_I,\gamma_J)$ for some partitioning $\{1,\cdots,n\}=I\cup J$. Then $\mathcal{L}$ is homogeneous with respect to the extensive variables q if and only if I is non-empty and $\widehat{F}(q_I,\gamma_J)$ is homogeneous of degree 1 in q_I. Furthermore, if $\mathcal{L}$ is homogeneous with respect to the extensive variables q, then*

$$\sum_{i=0}^n q_i p_i=0, \quad \textit{for all } (q,p)\in\mathcal{L} \tag{71}$$

Proof. As mentioned above, the first statement follows from the same reasoning as in Proposition 3.4, swapping the p and q variables. Equivalence of homogeneity of $\mathcal{L}$ with respect to q to $\widehat{F}(q_I,\gamma_J)$ being homogeneous of degree 1 in q_I directly follows from the expression of $\mathcal{L}$ in (27) in case $I\neq\emptyset$, while clearly homogeneity of $\mathcal{L}$ fails if $I=\emptyset$. Finally, if both $\alpha=\sum_{i=0}^n p_i dq_i$ and $\beta=\sum_{i=0}^n q_i dp_i$ are zero on $\mathcal{L}$, then $d(\sum_{i=0}^n q_i p_i)$ is zero on $\mathcal{L}$. Hence $\sum_{i=0}^n q_i p_i$ is constant on $\mathcal{L}$. Since $Z=\sum_{i=0}^n p_i\frac{\partial}{\partial p_i}$ is tangent to $\mathcal{L}$ this constant is necessarily zero. ∎

[6] Homogeneity with respect to the extensive variables can be generalized to *manifolds* $\mathcal{Q}$ using the theory developed in [25].

Remark 5.3. In a contact-geometric setting, an identity similar to (71) was noticed in [22]. A related scenario, explored in [9], is the case that $\mathcal{L}$ is a Lagrangian submanifold which is *non-mixing*: there exists a partitioning $\{0, 1, \cdots n\} = I \cup J$ such that $q_J = q_J(q_I)$, $p_I = p_I(p_J)$ for all $(q_I, q_J, p_I, p_J) \in \mathcal{L}$. Then $\mathcal{L}$ being Lagrangian amounts to

$$\frac{\partial q_J}{\partial q_I} = -\left(\frac{\partial p_I}{\partial p_J}\right)^\top \tag{72}$$

Since the left-hand side only depends on q_I and the right-hand side only on p_J, this means that both sides are *constant*, implying that $q_J = Aq_I$, $p_I = -A^\top p_J$ for some matrix A. Hence $\mathcal{L}$ is obviously satisfying (71), and is actually the product of two orthogonal *linear* subspaces; one in $\mathcal{Q} = \mathbb{R}^{n+1}$ and the other in the dual space $\mathcal{Q}^* = \mathbb{R}^{n+1}$.

Homogeneity of $\mathcal{L}$ with respect to the extensive variables q has the following classical implication. Start again with the case of a generating function $F(q, p) = -p_0\widehat{F}(q_1, \cdots, q_n)$ for $\mathcal{L}$, with q_0 being the energy variable. Since $\widehat{F}$ is homogeneous of degree 1 we may define for $q_1 \neq 0$

$$\bar{F}(\epsilon_2, \cdots, \epsilon_n) := \widehat{F}(1, \frac{q_2}{q_1}, \cdots, \frac{q_n}{q_1}) = \frac{1}{q_1}\widehat{F}(q_1, \cdots, q_n),\ \epsilon_j := \frac{q_j}{q_1},\ j = 0, 2, \cdots, n \tag{73}$$

Equivalently, $\widehat{F}(q_1, \cdots, q_n) = q_1\bar{F}(\epsilon_2, \cdots, \epsilon_n)$, where the function $\bar{F}$ is known in thermodynamics as the *specific energy* [24].

Geometrically this means the following. By homogeneity with respect to the p-variables the Liouville submanifold $\mathcal{L} \subset \mathcal{T}^*\mathbb{R}^{n+1}$ is projected to the Legendre submanifold $\widehat{\mathcal{L}} \subset \mathbb{R}^{n+1} \times \mathbb{P}(\mathbb{R}^{n+1})$, where $\mathbb{P}(\mathbb{R}^{n+1})$ is the n-dimensional projective space. Subsequently, by homogeneity with respect to the q-variables $\widehat{\mathcal{L}} \subset \mathbb{R}^{n+1} \times \mathbb{P}(\mathbb{R}^{n+1})$ is projected to a submanifold $\bar{\mathcal{L}} \subset \mathbb{P}(\mathbb{R}^{n+1}) \times \mathbb{P}(\mathbb{R}^{n+1})$. In coordinates the expression of $\bar{\mathcal{L}}$ is given as follows. Start from the expression of $\widehat{\mathcal{L}}$ as given in (27). Using the identities

$$\begin{aligned}
&q_0 = q_1\bar{F}(\epsilon_2, \cdots, \epsilon_n) \Leftrightarrow \epsilon_0 = \bar{F}(\epsilon_2, \cdots, \epsilon_n)\\
&\gamma_1 = \tfrac{\partial \widehat{F}}{\partial q_1} = \bar{F}(\epsilon_2, \cdots, \epsilon_n) - q_1\textstyle\sum_{\ell=2}^n \tfrac{\partial \bar{F}}{\partial \epsilon_\ell}\tfrac{q_\ell}{q_1^2} = \bar{F}(\epsilon_2, \cdots, \epsilon_n) - \textstyle\sum_{\ell=2}^n \epsilon_\ell \tfrac{\partial \bar{F}}{\partial \epsilon_\ell}\\
&\gamma_j = \tfrac{\partial \widehat{F}}{\partial q_j} = \tfrac{\partial(q_1\bar{F})}{\partial q_j} = \tfrac{\partial \bar{F}}{\partial \epsilon_j}, \quad j = 2, \cdots, n
\end{aligned} \tag{74}$$

the description (27) amounts to

$$\begin{aligned}
&\bar{\mathcal{L}} = \{(\epsilon_0, \epsilon_2, \cdots, \epsilon_n, \gamma_1, \cdots, \gamma_n) \mid \epsilon_0 = \bar{F}(\epsilon_2, \cdots, \epsilon_n),\\
&\gamma_1 = \bar{F}(\epsilon_2, \cdots, \epsilon_n) - \textstyle\sum_{\ell=2}^n \epsilon_\ell \tfrac{\partial \bar{F}}{\partial \epsilon_\ell},\ \gamma_2 = \tfrac{\partial \bar{F}}{\partial \epsilon_2}, \cdots, \gamma_n = \tfrac{\partial \bar{F}}{\partial \epsilon_n}\},
\end{aligned} \tag{75}$$

where

$$F(q, p) = -p_0\widehat{F}(q) = -p_0q_1\bar{F}(\epsilon_2, \cdots, \epsilon_n), \quad \epsilon_j := \frac{q_j}{q_1},\ j = 0, 2, \cdots, n \tag{76}$$

Similar expressions hold in the general case where the generating function for $\widehat{\mathcal{L}}$ is given by $\widehat{F}(q_I, \gamma_J)$ for some partitioning $\{1, \cdots, n\} = I \cup J$.

Furthermore, if the state properties captured by $\mathcal{L}$ are homogeneous with respect to q, it is natural to require the dynamics to be homogeneous with respect to q as well. Thus one requires the Hamiltonian $K(q, p)$ governing the dynamics to be homogeneous of degree 1, not only with respect to p, but also with respect to q, i.e.,

$$K(\mu q, p) = \mu K(q, p), \quad \text{for all } 0 \neq \mu \in \mathbb{R} \tag{77}$$

Equivalently (analogously to Proposition 3.7) one requires X_K to satisfy

$$\mathbb{L}_{X_K}\beta = 0 \tag{78}$$

Similarly to Proposition 3.8, this implies

$$[X_K, W] = 0, \quad W = \sum_{i=0}^n q_i\frac{\partial}{\partial q_i} \tag{79}$$

Hence the flow of X_K commutes both with the flow of the Euler vector field $Z = \sum_{i=0}^n p_i\frac{\partial}{\partial p_i}$ and with the vector field $W = \sum_{i=0}^n q_i\frac{\partial}{\partial q_i}$.

We have seen before that projection of X_K along Z yields the contact vector field $X_{\widehat{K}}$, with $K(q, p) = -p_0\widehat{K}(q, \gamma)$, $\gamma_j = \frac{p_j}{-p_0}$, $j = 1, \cdots, n$, where $(q, \gamma) \in \mathbb{R}^{n+1} \times \mathbb{P}(\mathbb{R}^{n+1})$. Subsequent projection along W to the reduced space $\mathbb{P}(\mathbb{R}^{n+1}) \times \mathbb{P}(\mathbb{R}^{n+1})$ can be computed as follows. First write as above

$$\widehat{K}(q,\gamma) = q_1 \bar{K}(\epsilon,\gamma), \quad \epsilon_j = \frac{q_j}{q_1}, \quad j = 0, 2, \cdots, n \tag{80}$$

Then compute, analogously to (30),

$$\begin{array}{ll} \frac{\partial \widehat{K}}{\partial q_1} = \bar{K} - \sum_{\ell=0,2}^{n} \epsilon_\ell \frac{\partial \bar{K}}{\partial \epsilon_\ell} & \\ \frac{\partial \widehat{K}}{\partial q_j} = \frac{\partial \bar{K}}{\partial \epsilon_j}, & j = 0, 2 \cdots, n \\ \frac{\partial \widehat{K}}{\partial \gamma_j} = q_1 \frac{\partial \bar{K}}{\partial \gamma_j}, & j = 1, \cdots, n \end{array} \tag{81}$$

Combining, analogously to (38), with the expression

$$\dot{\epsilon}_j = \frac{\dot{q}_j}{q_1} - \frac{q_j}{q_1^2}\dot{q}_1, \tag{82}$$

this yields the following $2n$-dimensional dynamics on the *reduced thermodynamic phase space* $\mathbb{P}(\mathbb{R}^{n+1}) \times \mathbb{P}(\mathbb{R}^{n+1})$

$$\begin{array}{lll} \dot{\epsilon}_j & = & \frac{\partial \bar{K}}{\partial \gamma_j} - \epsilon_j \left(\sum_{\ell=1}^{n} \gamma_\ell \frac{\partial \bar{K}}{\partial \gamma_\ell} - \bar{K} \right), \qquad j = 0, 2, \cdots, n \\ \dot{\gamma}_j & = & -\frac{\partial \bar{K}}{\partial \epsilon_j} + \gamma_j \left(\sum_{\ell=0,2}^{n} \epsilon_\ell \frac{\partial \bar{K}}{\partial \epsilon_\ell} - \bar{K} \right), \quad j = 1, 2 \cdots, n, \end{array} \tag{83}$$

where $\bar{K}$ is determined by

$$K(q,p) = -p_0 q_1 \bar{K}(\epsilon,\gamma), \quad \epsilon = \left(\frac{q_0}{q_1}, \frac{q_2}{q_1} \cdots, \frac{q_n}{q_1} \right), \ \gamma = \left(\frac{p_1}{-p_0}, \cdots, \frac{p_n}{-p_0} \right) \tag{84}$$

Obviously, if q_0 represents *entropy* the same expressions hold with different interpretation of $\epsilon_0, \epsilon_2, \cdots, \epsilon_n$. Note that (83) consists of standard Hamiltonian equations with respect to the Hamiltonian $\bar{K}$, together with extra terms. In view of (54), the first part of these extra terms resulting from $\bar{K}^a$, i.e., $\sum_{\ell=1}^{n} \gamma_\ell \frac{\partial \bar{K}^a}{\partial \gamma_\ell} - \bar{K}^a$, is zero on $\mathcal{L}$.

The precise geometric interpretation of the $2n$-dimensional dynamics (83) is an open question. It can be noted that while the above reduction from $\mathcal{L}$ and X_K to $\bar{\mathcal{L}}$ and the dynamics (83) has been performed via $\widehat{\mathcal{L}}$ and $X_{\widehat{K}}$ (the contact-geometric description on the thermodynamic phase space), the same outcome would have been obtained by instead *first* projecting onto $\mathbb{P}(\mathbb{R}^{n+1}) \times \mathbb{R}^{n+1}$ along W, and *then* projecting onto $\mathbb{P}(\mathbb{R}^{n+1}) \times \mathbb{P}(\mathbb{R}^{n+1})$ along Z. Said otherwise, this alternative route involves a *different* intermediate contact geometric description on the contact manifold $\mathbb{P}(\mathbb{R}^{n+1}) \times \mathbb{R}^{n+1}$ with coordinates $\epsilon_0, \epsilon_2, \cdots, \epsilon_n, p_0, \cdots, p_n$. This double fiber bundle structure could be instrumental in the investigation of the geometric structure of (83).

6. Conclusions

The geometric formulation of classical thermodynamics gives rise to a specific branch of symplectic geometry, coined as *Liouville geometry*, which is closely related to contact geometry [2,3,25]. A detailed treatment of Liouville submanifolds and their generating functions has been provided. The same has been done for homogeneous Hamiltonian vector fields, extending the treatment in e.g. [2,3,25]. We refer to [37] for the formulation of the Weinhold and Ruppeiner metrics in the Liouville geometry setting. The interpretation of the resulting Hamiltonian formulation of port-thermodynamic systems turns out to be rather different from Hamiltonian formulations of other parts of physics such as mechanics. In particular, the state properties of the thermodynamic system define a Liouville submanifold, which is left invariant by the Hamiltonian dynamics. Furthermore, the Hamiltonian is *dimensionless*, while its corresponding contact Hamiltonians have dimension of power (in the energy representation) or of entropy flow (in the entropy representation). An open modeling problem concerns the determination of the Hamiltonian governing the dynamics. A partial answer is provided in [37], where it is shown how the Hamiltonian of a thermodynamic system can be derived from the Hamiltonians of the constituent subsystems. In Section 5 another type of homogeneity has been considered; this time with respect to the extensive variables, corresponding to the classical Gibbs-Duhem relation. It has been shown how this gives rise to a projection on the product of the n-dimensional projective space with itself. The precise geometric interpretation and properties of the reduced dynamics (83) warrant further study.

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Declaration of competing interest

None.

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